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EIGENVALUE OF A MODEL CHEMICAL
REACTION,

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OF A MODEL CHEMICAL REACTION

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ABSTRACT

In this paper we analyze the steady-state bifurcations from the trivial
solution of the reaction-diffusion equations associated to a model chemical
reaction, the so-called Brusselator. The present analysis concentrates
on the case when the first bifurcation is from a double eigenvalue. The
dependence of the bifurcation diagrams on various parameters and perturba-
tions is analyzed. The results of Technical Summary Report #1844 are
invoked to show that further complications in the model would not lead to
new behavior.

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SIGNIFICANCE AND EXPLANATION

It is believed that pattern formation by biological systems may be related to repeated bifurcations of the reaction-diffusion equations governing the concentrations of the various chemicals present in the system. The full complexity that these equations can exhibit is far from understood. Here we take an initial step in this direction by analyzing the bifurcations of a model chemical reaction, the so-called tri-molecular model of Lefever and Prigogine, at and near a double eigenvalue. The dependence of this system on various parameters and its sensitivity to perturbations is also studied.

This paper differs from earlier work in several points. First we apply the notion of universal unfoldings (developed in MRC Technical Summary Report #1844) to show that no qualitatively new behavior would result from the addition of further perturbations in the model. Second, we show that symmetry plays a dominant role in determining the behavior of the system, a fact that seems to have escaped notice. Finally we have been able to attain a higher level of rigor than previous work on double eigenvalues.

BIFURCATION ANALYSIS NEAR A DOUBLE EIGENVALUE OF A MODEL CHEMICAL REACTION

David G. Schaeffer[1] and Martin A. Golubitsky[2]

§1. Discussion of the problem

In this paper we consider the one-dimensional reaction-diffusion equations associated to the so called tri-molecular model of Lefever and Prigogine [6], less formally known as the "Brusselator". For the parameter range in which we are interested, this system exhibits bifurcation from a spatially and temporally homogeneous solution into steady-state, spatially inhomogeneous solutions. The first bifurcation may be from either a simple or a double eigenvalue. A number of authors [1,5] have discussed the case of a simple eigenvalue, but rather less seems to be known about the non-simple case. Here we analyze the bifurcations of this system at the double eigenvalues as an application of the theory developed in [2,3]. We obtain a rather complete classification of the possible bifurcation diagrams in the vicinity of such points. Some of our results were obtained earlier by Keener [5a] by less rigorous methods - his results are compared with ours at the end of §1.

The relevant equations for this model are

$$(1.1) \quad \begin{cases} \dfrac{\partial X}{\partial t} = D_1 \dfrac{\partial^2 X}{\partial \xi^2} + X^2 Y - (B + 1)X + A \\[2em] \dfrac{\partial Y}{\partial t} = D_2 \dfrac{\partial^2 Y}{\partial \xi^2} - X^2 Y + BX \end{cases}$$

subject to boundary conditions of Dirichlet type

$$(1.2) \quad X(0) = X(\pi) = A, \quad Y(0) = Y(\pi) = B/A .$$

Here the unknown functions X and Y are chemical concentrations, A and B are constant, externally controlled concentrations, and D_1, D_2 are diffusion coefficients. B plays the role of the bifurcation parameter; that is, we are interested in the

bifurcation of new solutions of (1.1), (1.2) from the trivial solution

(1.3) $X = A, \qquad Y = B/A$

as B is increased. To facilitate the analysis we define incremental variables

$$u = X - A, \qquad v = Y - B/A ,$$

for which we use the vector notation $w = (u,v)$. These variables satisfy the equation

(1.4) $$\frac{\partial w}{\partial t} = Lw + N(w)$$

where

(1.5) $$L = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix} \frac{\partial^2}{\partial \xi^2} + \begin{pmatrix} B - 1 & A^2 \\ -B & -A^2 \end{pmatrix}$$

and

(1.6) $$N(w) = \left(\frac{B}{A} u^2 + 2Auv + u^2 v \right) \begin{pmatrix} 1 \\ -1 \end{pmatrix} .$$

Both time independent and time periodic solutions of (1.4) can bifurcate from the zero solution of this equation, depending on the various parameters. However if D_2 is rather larger than D_1, say D_2/D_1 is at least 3, then the first bifurcation gives a time independent solution. (See [1] for proofs.) We consider only this case.

Bifurcation of a steady state solution of (1.4) can only occur if the linear operator L in (1.5) is singular. To avoid confusion let us say explicitly that L operates on $C^0([0,\pi], \mathbb{R}^2)$ with homogeneous Dirichlet boundary conditions. Since L commutes with $(\partial/\partial \xi)^2$, the eigenfunctions of L may be sought in the form

(1.7) $$\sin \ell\xi \begin{pmatrix} a \\ b \end{pmatrix}$$

where a, b are constants and ℓ is an integer. The two eigenvalues of L associated to eigenfunctions of the form (1.7) are eigenvalues of the matrix

(1.8) $$\begin{pmatrix} B - 1 - \ell^2 D_1 & A^2 \\ -B & -A^2 - \ell^2 D_2 \end{pmatrix} .$$

Zero is an eigenvalue of (1.8) if and only if $B = B_\ell$, where

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(1.9)
$$B_\ell = 1 + \frac{D_1}{D_2} A^2 + D_1 \ell^2 + \frac{A^2}{D_2 \ell^2} .$$

Thus the first bifurcation point of (1.4) is given by

(1.10)
$$\min_\ell B_\ell .$$

For most values of the parameters in the problem this minimum will be achieved for exactly one value of ℓ, and then the first bifurcation will be from a simple eigenvalue. However if

(1.11)
$$A^2 = D_1 D_2 k^2 (k + 1)^2$$

for some integer k, then the minimum in (1.10) is achieved at both $\ell = k$ and $\ell = k + 1$, and the eigenvalue is double. In other words, when the zero solution of (1.4) first loses stability, it loses stability simultaneously with respect to disturbances of wave number k and of wave number $k + 1$. This is the case we study in the present paper.

Our task of analyzing the bifurcations of (1.1), (1.2) near a double eigenvalue may be conveniently divided into two steps. It turns out that (in non-degenerate cases) either one or three new solutions bifurcate from the trivial solution at a double eigenvalue, and various combinations of stability or instability for the new solutions are possible. In all there are five different cases. Our first problem is to determine which case occurs as a function of the parameters A, D_1, D_2. (Only two of these are really independent, as the requirement that a double eigenvalue occur leads to the condition (1.11).) The second step in the analysis is to study the effect of various perturbations on the bifurcation. There are two natural perturbations to consider in this connection. One is to change A, D_1, D_2 from unperturbed values which satisfy (1.11) exactly to perturbed values which satisfy (1.11) only approximately. Observe that, no matter what the values of these parameters, (1.3) still provides a spatially and temporally homogeneous solution of (1.1), (1.2). The effect of this perturbation is to split the double eigenvalue, so that two separate bifurcations from

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the trivial solution occur, both at simple eigenvalues. This perturbation induces secondary bifurcation away from the trivial solution. The other perturbation we consider is to replace the parameter A in (1.1) by the function

$$(1.12) \qquad A(\xi) = A_0 \frac{\cosh\sqrt{\epsilon} \ (\xi - \frac{\pi}{2})}{\cosh\sqrt{\epsilon} \ \frac{\pi}{2}} \ ,$$

which is motivated by the following considerations. In the derivation of (1.1) it is assumed that A measures a chemical concentration which is fixed by the experimenter. In practice concentrations can only be fixed at the boundary of the domain; in the interior the concentrations will be determined by solving a boundary problem

$$\frac{\partial^2 A}{\partial \xi^2} - \epsilon A = 0 \quad \text{on} \quad (0, \pi)$$

$$A(0) = A(\pi) = A_0 \ ,$$

which has solution (1.12). Here ϵ measures the rate at which A is depleted relative to its diffusivity. When $\epsilon = 0$, (1.12) reduces to the previous case, but when $\epsilon > 0$ an explicit, trivial solution of (1.1) analogous to (1.3) is no longer available. Indeed, as a result of this perturbation there may exist a range of B where (1.1) has no steady state solutions, spatially homogeneous or otherwise, at least not in the neighborhood of (1.3). The effect of this perturbation is similar to the effect of imperfections on bifurcation at a simple eigenvalue. (See for example [2,9].)

There is an important symmetry present in (1.4) that restricts considerably the possible behavior in this problem. Namely (1.4) commutes with the reflection

$$(1.13) \qquad\qquad Rw(\xi) = w(\pi - \xi) \ .$$

In other words, no change in (1.4) occurs if one makes a coordinate transformation $\xi' = \pi - \xi$ which interchanges right and left endpoints of the interval. Observe that

$$R \sin \ell\xi = (-1)^{\ell+1} \sin \ell\xi \ .$$

Thus one of the two eigenfunctions of L at the double eigenvalue is even and one is odd. The two perturbations of the problem mentioned above also commute with (1.13).

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We study the equilibrium equation associated to (1.4), namely

(1.14) $Lw + N(w) = 0$,

by means of the Lyapunov-Schmidt reduction. (See §4 for details.) At a double eigen-
value this procedure reduces (1.14) to a system of two equations in two unknowns,
depending on a parameter. Let us write the reduced equations

(1.15) $\underline{G}(\underline{x},\lambda) = 0$

where $\underline{G} : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$. Here $\underline{x} = (x,y)$ parametrizes the kernel of L and
$\lambda = B - B_0$, where B_0 is the bifurcation point. Our notation in (1.15) does not
indicate explicitly the other parameters in the problem. We will show below that at a
double eigenvalue the reduced equations may be written

(1.16) $\underline{G}(\underline{x},\lambda) = \begin{pmatrix} x^2 + \eta y^2 + \lambda x \\ cxy + \lambda y \end{pmatrix}$,

where $c \in \mathbb{R}$ and $\eta = \pm 1$. (This equation holds   to cubic terms, and in non-
degenerate cases the cubic terms may be transformed   change of coordinates.)
The symmetry of (1.14) with respect to the transformation   is reflected in the
fact that the first component of (1.16) is even with respect to y while the second
is odd. Thus the bifurcation diagram

(1.17) $\{(\underline{x},\lambda) \in \mathbb{R}^2 \times \mathbb{R} : \underline{G}(\underline{x},\lambda) = 0\}$

is invariant under the reflection $y \mapsto -y$.

The first step in our analysis is to compute the coefficients c and η in (1.16)
as functions of the various parameters in the problem. It is then a simple matter to
determine the type of the bifurcation diagram by invoking the classification results
of [3]. (Strictly speaking to obtain the stability properties of the bifurcating solu-
tions the arguments of [3] must be supplemented, which is done in §§6 and 7 of the
present paper.) This solves our first problem, that of describing the bifurcation
diagrams at the double eigenvalue proper. For the perturbed problems we again refer
to [3], this time for a result that an arbitrary small, symmetry preserving perturbation
of (1.16) may be described, up to a certain equivalence, by two parameters. In more

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technical language, an appropriate universal unfolding of (1.16) requires two parameters.
(See §3 for greater detail.) The fact that two parameters suffice depends strongly
on the presence of the symmetry (1.13) - without this, five parameters would be
required [2]. The two parameters of the universal unfolding may be identified with the
two perturbations of the physical problem discussed above. The fact that two parameters
suffice for the unfolding means that additional perturbations of (1.4) - one might
for example treat B as a variable concentration, partially depleted in the interior,
or one might consider boundary conditions other than (1.2) - would not lead to more
complicated behavior than that already obtainable with the two perturbations considered.

This paper has much in common with Keener [5a], a reference kindly brought to our
attention by W. H. Ray. We feel that our paper sheds new light on the subject on
several accounts, quite apart from questions of rigor. Perhaps most important, the
existence of a universal unfolding with a known, finite number of unfolding parameters
ensures that the sort of parameter exploration undertaken in these papers is a terminat-
ing process - although new complications may be introduced into the model indefinitely,
no qualitatively new behavior will result after the parameters of the universal unfold-
ing are represented. Secondly, the present paper emphasizes the importance of symmetry
in this problem, without which a number of qualitatively new phenomena could occur.
For example the occurrence of secondary bifurcation depends on symmetry. Consider a
perturbation of the reduced equation (1.16) of the form

(1.17a) $\underline{G}(\underline{x},\lambda) + M\underline{x}$,

where M is a 2×2 matrix. Such perturbations do not affect the existence of the
trivial solution $x = 0$ but (in general) do split the double eigenvalue. It can be
shown that if, say $c < 0$ and $\eta = +1$, then secondary bifurcation occurs for the
perturbed problem if and only if M is upper triangular (non-zero diagonal entries
permitted). Here bifurcation means the crossing of solution branches, not merely the
existence of a limit point. The first perturbation discussed above, namely moving
A, D_1, D_2 slightly away from values satisfying (1.11), may be represented in the form
(1.17a), where however the fact that the perturbation preserves symmetry implies that

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M is diagonal. In particular M is upper triangular, so secondary bifurcation does occur. Of course for a symmetry breaking perturbation no such special form may be expected. A final difference between [5a] and the present paper is that we consider the two distinct perturbations - Keener does not consider (1.12). From our point of view it is natural to try to find physical representations for both of the unfolding parameters in the universal unfolding, not to mention the considerable physical interest of (1.12).

The following notation will be used throughout this paper. Let $\theta = D_2/D_1$ and let $\bar{A} = \theta^{-\frac{1}{2}} A$. Equation (1.11) may be re-written

(1.18)
$$\bar{A} = k(k + 1)D ,$$

where D without a subscript indicates D_1. In Figure 1.1 the lines labeled $(k, k + 1)$ indicates the lines in the $(\bar{A}, D)$ plane where (1.18) is satisfied. Between the lines $(k - 1, k)$ and $(k, k + 1)$ the first eigenvalue is simple and the associated eigenfunction has spatial dependence $\sin k\xi$. If (1.18) is satisfied, the first bifurcation occurs when

(1.19)
$$B = (1 + D\mu_1)(1 + D\mu_2) ,$$
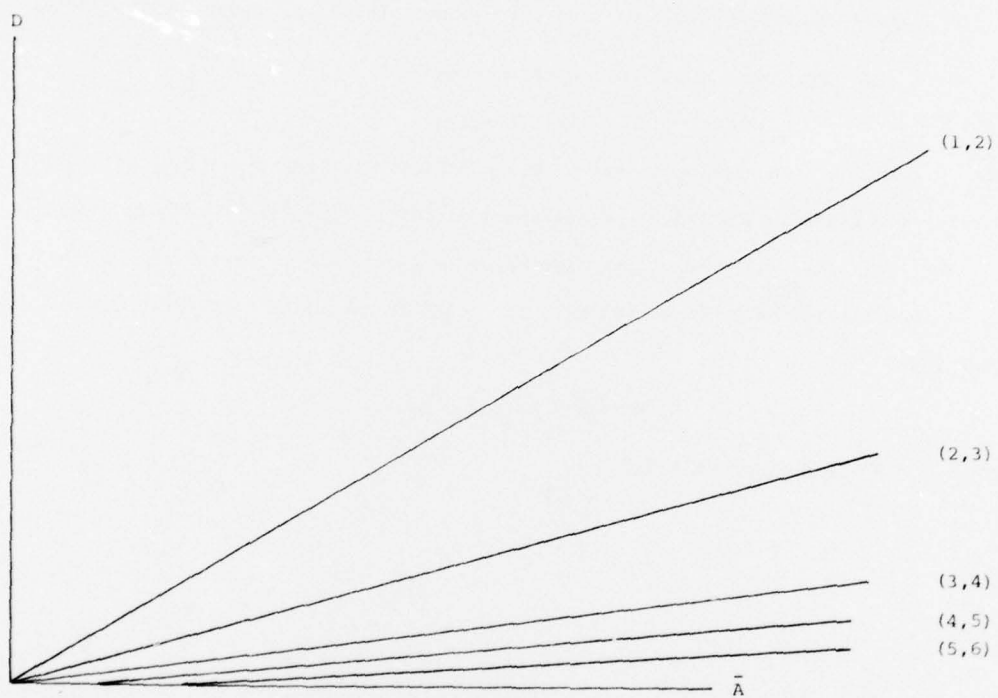
where $\mu_1 = k^2$ and $\mu_2 = (k + 1)^2$.

Figure 1.1

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§2. Statement of results

In this section we present our main results, deferring the proofs for later sections. Illustrations of the bifurcation diagrams, as defined by (1.17), offer the most convenient format for this presentation. Some comments about Figures 2.2-4 below may help in their interpretation. These figures are intended to represent three dimensional bifurcation diagrams, the three coordinates being λ, the bifurcation parameter; x, the amplitude of the eigenfunction whose profile is symmetric with respect to (1.13); and y, the amplitude of the anti-symmetric eigenfunction. The orientation of these coordinates shown in Figure 2.2 is retained throughout. The "Y" or diamond shaped figure at the ends of some of these bifurcation diagrams is intended as an aid to visualization and does not represent part of the diagram itself. In Figure 2.2 we have shown the bifurcation diagrams of the unperturbed problem as a union of straight lines through the origin. Here "T" denotes the trivial solution, which coincides with the λ-axis. The branches labeled T and 1 span the plane of symmetry $\{y = 0\}$, while branches 2 and 3, when present, are located symmetrically in a plane $\{cx + \lambda = 0\}$ perpendicular to the plane of symmetry. (Cf (1.16).) In the perturbed diagrams, Figures 2.3 and 2.4, we have labeled the solution branches far away from the bifurcation point by the closest solution branch of the unperturbed problem. In all cases the perturbed diagram consists of two conic sections, the branches T and 1 lying in the plane $\{y = 0\}$, the other branches lying symmetrically in a plane $\{cx + \lambda = \text{const}\}$.

In our bifurcation diagrams the various solution branches have stability assignments determined by the spectrum of the linearized equation. We claim that at most two eigenvalues of the linearized equations lie in the unstable (right) half plane - this follows by perturbation theory from the observation that the unperturbed problem has a double eigenvalue at zero and the remainder of its spectrum lies in a half plane $\{\zeta : R\ell\zeta \leq -\epsilon\}$, where $\epsilon > 0$. In the figures we indicate the three cases of zero, one, or two eigenvalues in the right half plane by labels +s, - , +u, respectively. Here the sign gives the Leray-Schander degree while the latter distinguishes between the stable and unstable cases with positive degree.

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We should caution the reader that our representation of the bifurcation diagrams is purely local. It is known [1] that for sufficiently small λ the solution of (1.4) is unique and that for λ bounded the solutions satisfy an a priori estimate. Thus the bifurcating solutions must turn around in the large, as indicated in Figure 2.5 for the unperturbed case I_0 (notation defined below).

First we consider the unperturbed case when (1.18) is satisfied exactly. As mentioned above, either one or three non-trivial solutions of (1.4) may bifurcate from the trivial solution at the double eigenvalue. If one new solution bifurcates, it may be either unstable or stable, while if three such bifurcate, either zero, one, or two of them may be stable. We refer to these cases as I_0, I_1, III_0, III_1, III_2 respectively - the Roman numeral indicates the number of bifurcating solutions and the subscript the number of them which are stable. It turns out that which case occurs depends on $\bar{A}$ and D but not on θ. The type of the bifurcation as a function of these two parameters may be determined from Figure 2.1, where we have identified two sets of five regions in the $\bar{A}$, D plane in which different behavior obtains. The two different partitions correspond to k odd or even. Equations for the boundaries of these regions are given in §4. We have sketched in Figure 2.2 bifurcation diagrams for each of the five cases. (In this paper we do not consider the degenerate cases when $(\bar{A}, D)$ lies on the boundary between two regions in Figure 2.1.)

We now consider the effects of changing the parameters $\bar{A}$ and D, the first of our two perturbations. (As above the bifurcation diagram does not depend on θ.) If $(\bar{A}, D)$ varies along one of the lines $(k, k+1)$ in Figure 2.1, no qualitative change in the bifurcation diagram will occur unless $(\bar{A}, D)$ crosses into a different region. (This is of course a local statement - the size of the neighborhood in which it is valid decreases as the boundary is approached.) Thus only one of these parameters has a qualitative effect on the nature of the bifurcation diagram. Let us take δ, the change in D. Making δ non-zero splits the double eigenvalue into two simple eigenvalues, causing secondary bifurcation. We illustrate the effect of this perturbation
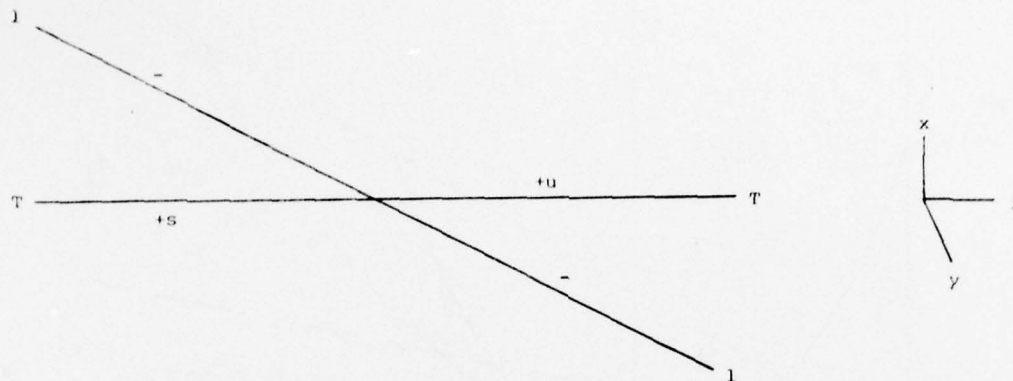
Figure 2.1

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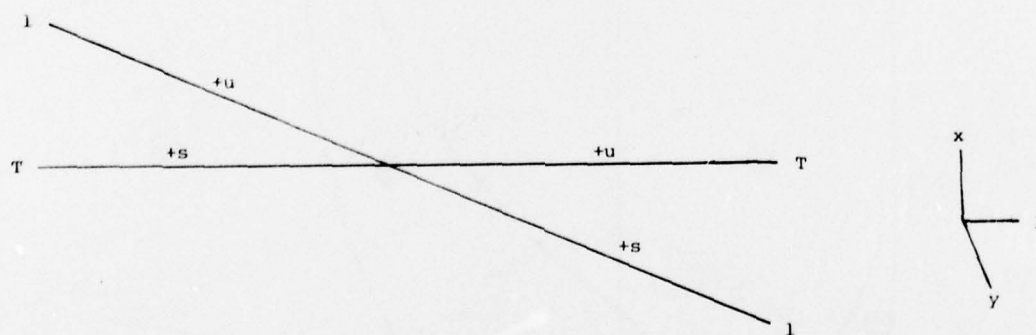Figure 2.2a: Unperturbed I_0

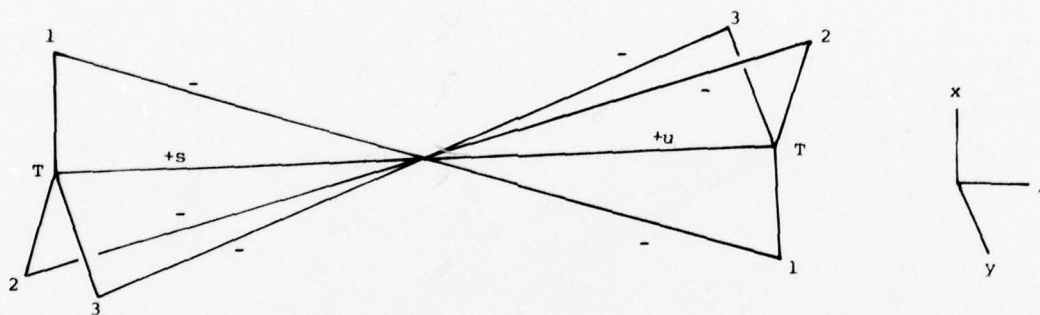Figure 2.2b: Unperturbed I_1
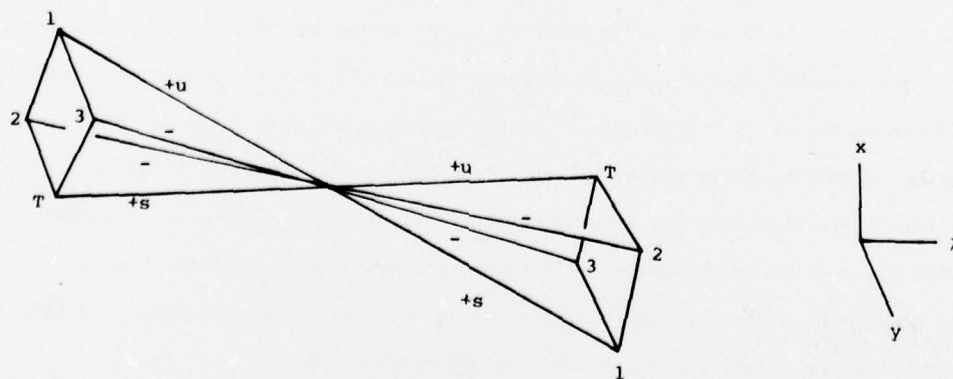
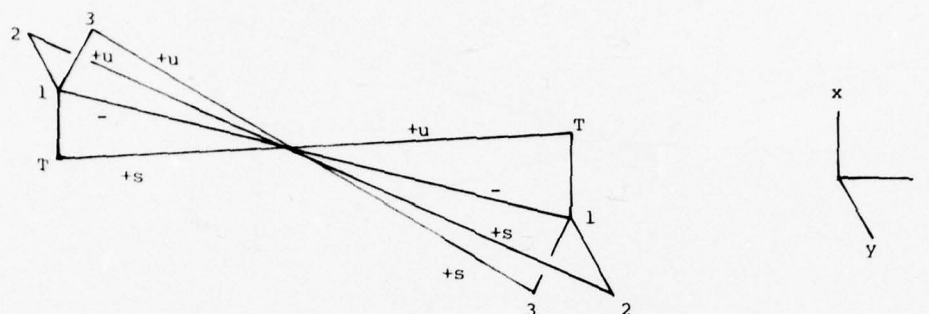Figure 2.2c: Unperturbed III_0

Figure 2.2d: Unperturbed III_1

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Figure 2.2e: Unperturbed III_2

for the five cases above in Figure 2.3. The diagram depends on the sign of δ and the parity of k as indicated. Note that the λ-axis, representing the trivial solution, is a part of all these diagrams. Of course the effect of the perturbation is strongest near the center of the diagram - although the perturbation is uniformly small through-out the interval, the unperturbed problem is rather singular near the double eigenvalue proper and hence more sensitive to perturbations. Perhaps the most noteworthy feature of these diagrams occurs in Figure $2.3b_1$. (Let us remark that the circle in this diagram lies in a plane perpendicular to the two lines. Similarly for Figure 2.3a.) The solution branch that originates from the first bifurcation exists only for a small interval above the bifurcation point before it is reabsorbed by a secondary bifurcation. A similar phenomenon occurs in Figure $2.3e_2$. It is also worth remarking that the first bifurcation can be either super-, trans-, or sub-critical.

As to the second perturbation, we have sketched in Figure 2.4 the bifurcation diagrams which result from taking $\varepsilon > 0$ in (1.12). The outcome depends on the region and on the parity of k in a somewhat confusing manner. For example, the unperturbed diagrams when $(\bar{A}, D)$ belongs to region 1 or 5, k odd or even, are all the same, namely III_1; above if $\delta \neq 0$ the perturbed diagram depends on the parity of k but not the region, while here if $\varepsilon > 0$ the diagram depends on the region but not the parity of k.

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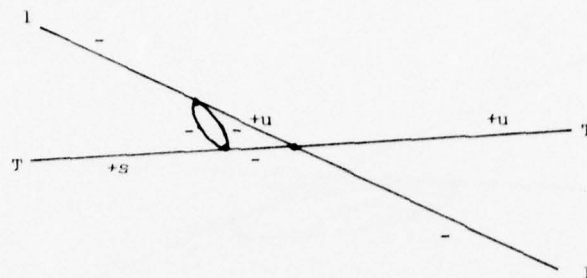Figure 2.3a$_1$: I_0, $(-1)^k \delta > 0$

Figure 2.3a$_2$: I_0, $(-1)^k \delta < 0$

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Figure 2.3b$_1$: I_1, $(-1)^k \delta > 0$

Figure 2.3b$_2$: I_1, $(-1)^k \delta < 0$
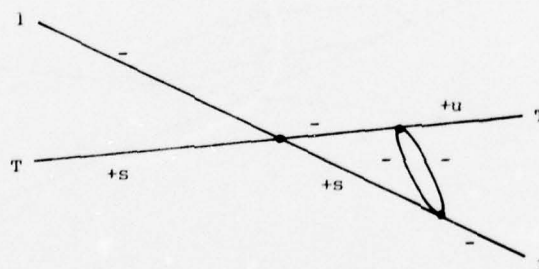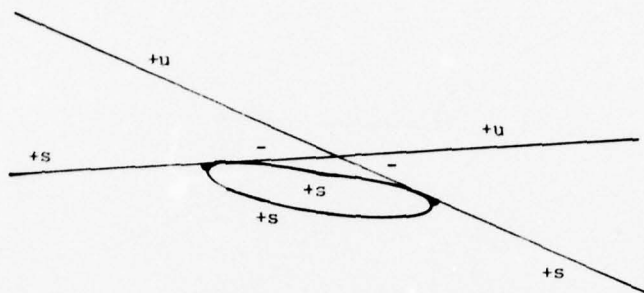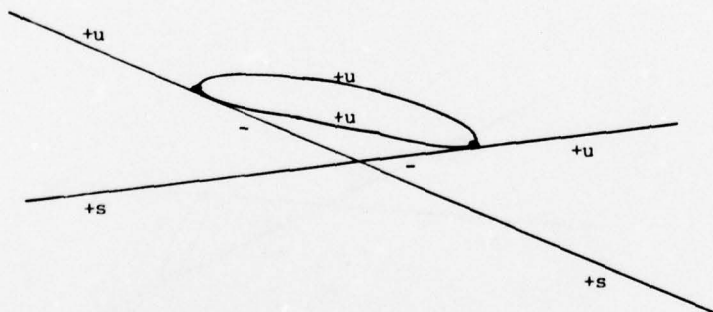
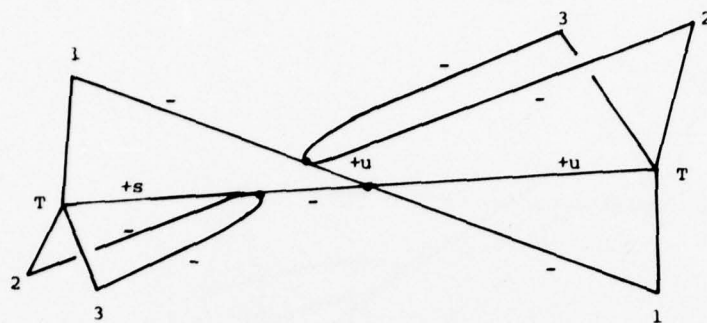Figure 2.3c$_1$: III_0, $(-1)^k \delta > 0$
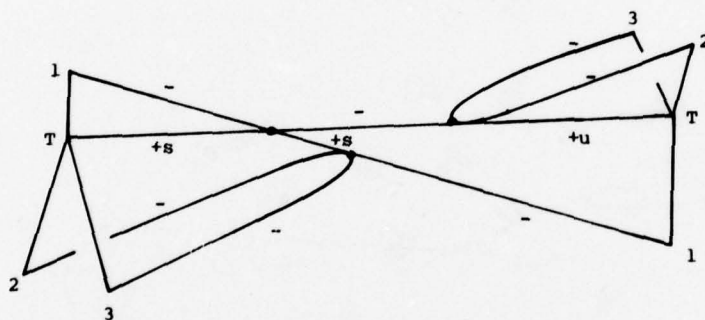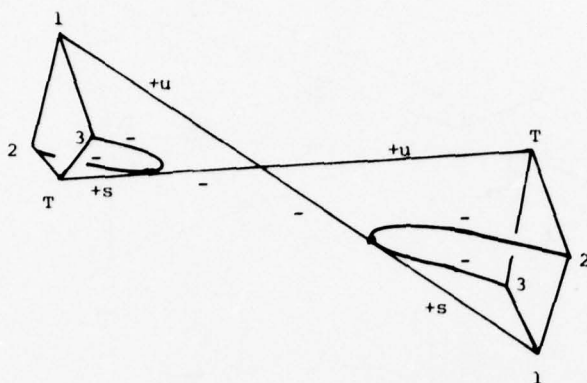
Figure 2.3c$_2$: III_0, $(-1)^k \delta < 0$

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Figure 2.3d$_1$:   III$_1$,(-1)$^k\delta > 0$

Figure 2.3d$_2$:   III$_1$,(-1)$^k\delta < 0$
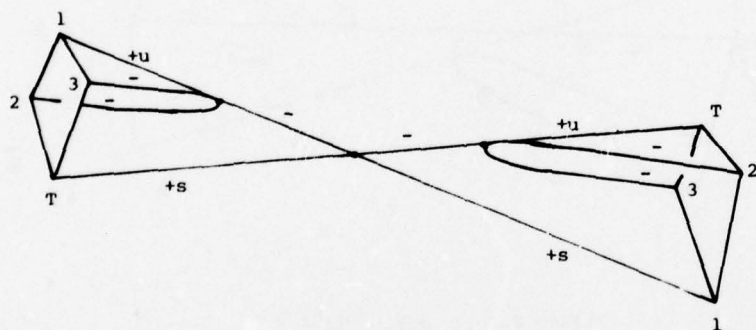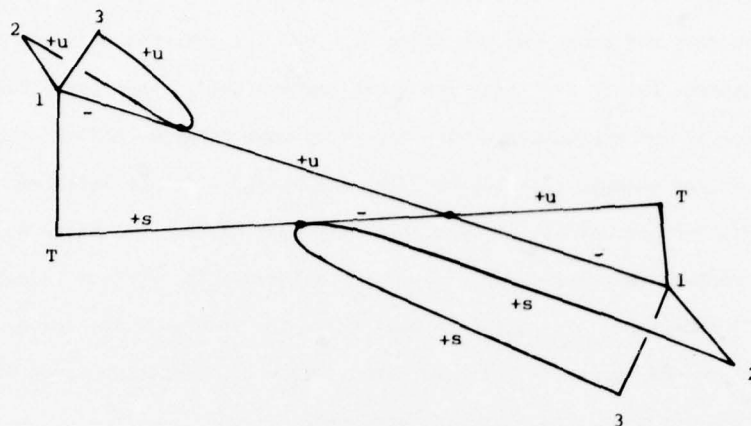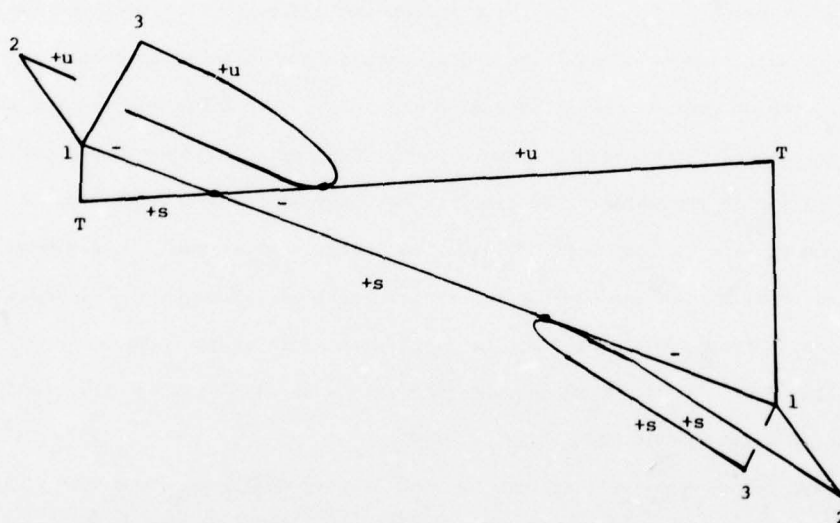
Figure 2.3e₁: III₂, $(-1)^k \delta > 0$

Figure 2.3e₂: III₂, $(-1)^k \delta < 0$

Negative values of ε would lack physical significance. As it happens, however, for the various unperturbed diagrams of type III, the diagram which would result if $\varepsilon < 0$ occur anyway for $(\bar{A}, D)$ in a different region and k of the opposite parity. This duplication does not occur for the cases I_0 or I_1. We have none the less included the diagrams for $\varepsilon < 0$ with the label "unphysical", since these diagrams could well appear if the perturbation were caused by some other mechanism without a definite sign, as for example imposing boundary conditions slightly different from (1.2). We do not analyze such possibilities here, but only mention that no matter how complicated the perturbing mechanism (assumed symmetric), the diagram which results is determined qualitatively by the values of the two parameters in the universal unfolding of (1.16). (See [2] concerning non-symmetric perturbations.) This consideration gives the diagrams here a greater significance than otherwise apparent.

By far the most interesting of these diagrams is that of Figure $2.4e_1$. (We caution the reader not to try to imagine a surface spanned by solution branches 1 and 2 or 1 and 3 – rather think of 2 and 3 as lying in a plane $cx + \lambda = 0$.) Here the two non-trivial solution branches of positive degree change from unstable to stable as λ is increased, without ever encountering a zero eigenvalue – in other words, they undergo a Hopf bifurcation! As mentioned above a Hopf bifurcation can sometimes occur from the trivial solution in the unperturbed problem, but only at much larger values of B; indeed the Hopf bifurcation of Figure $2.4e_1$ can occur for parameter values where the unperturbed problem does not admit any Hopf bifurcations. Because the eigenvalues must be close to zero, the period of the associated limit cycles will be large, specifically $O(\varepsilon^{-1/2})$. In a subsequent publication we will consider the stability and the domain of existence of these limit cycles.

Finally, let us suppose that both δ and ε are non-zero. Then there exist six regions of the δ, ε plane where the perturbed diagrams exhibit different structure, as indicated in Figure 2.6 for the case III_0. Note that regions 1, 2, 4, and 5 in the figure only contain points (δ, ε) for which $\varepsilon = O(\delta^2)$. We feel that regions 3 and 6

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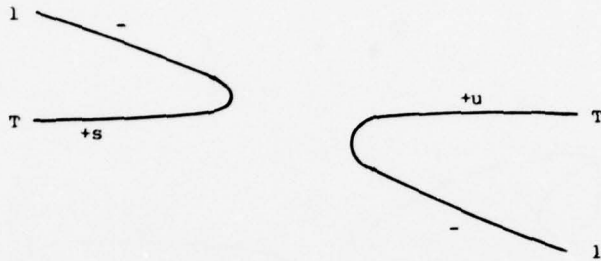
Figure 2.4a$_1$:   I$_0$, ε > 0
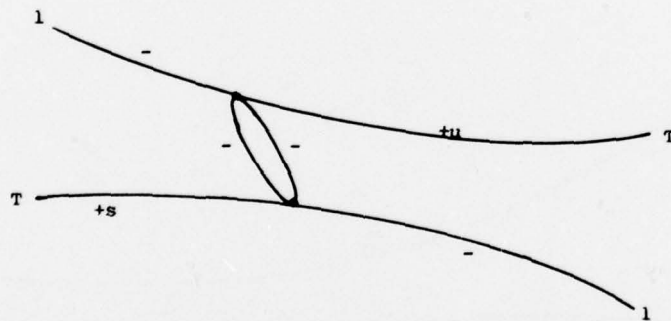
Figure 2.4a$_2$:   I$_0$, unphysical
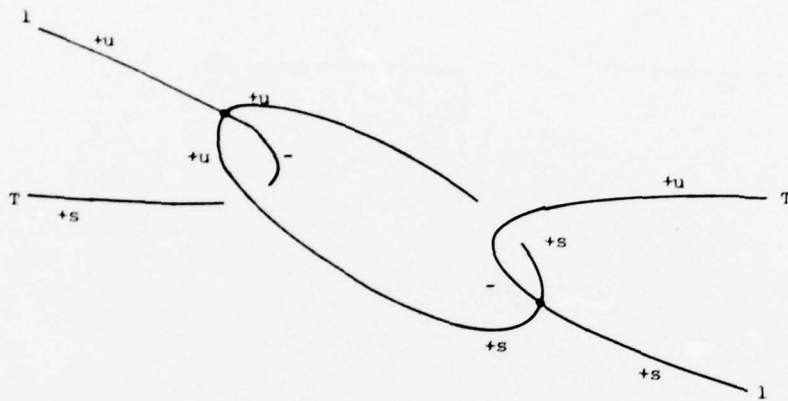
Figure 2.4b$_1$: I$_1$, unphysical

Figure 2.4b$_2$: I$_1$, $\varepsilon > 0$

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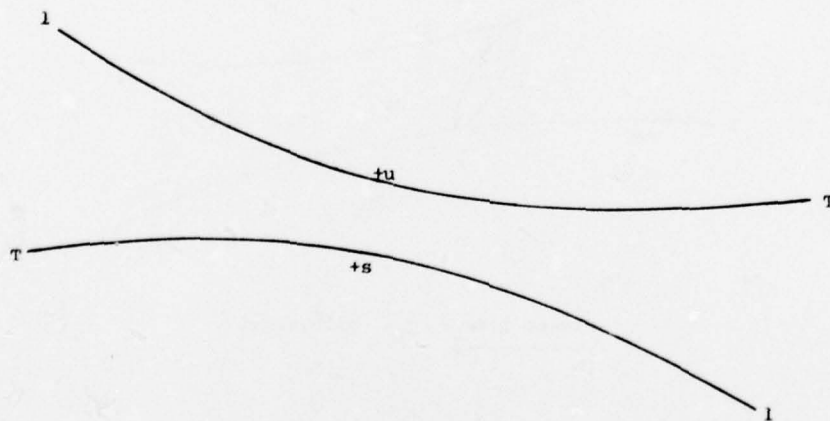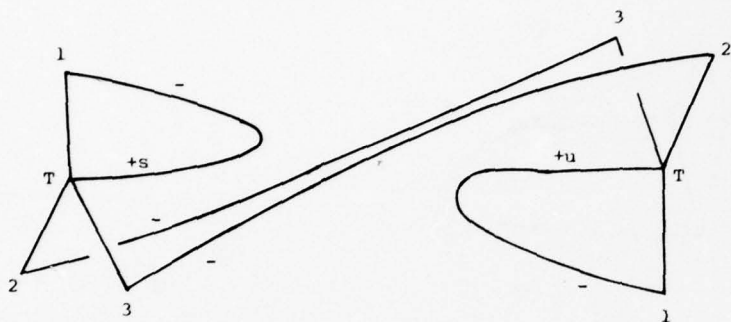
Figure 2.4c$_1$:   III$_0$, $\varepsilon > 0$, k even
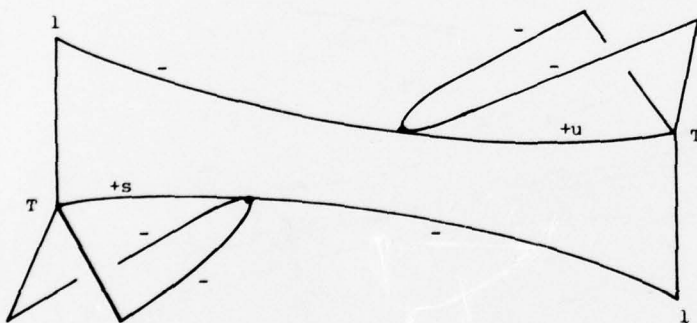
Figure 2.4c$_2$:   III$_0$, $\varepsilon > 0$, k odd
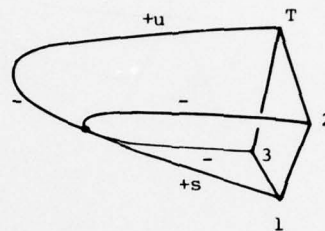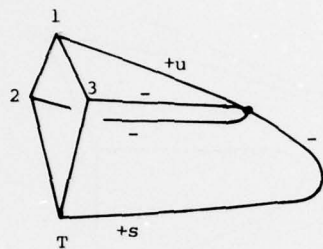
Figure 2.4d$_1$: III$_1$, $\varepsilon > 0$, region 5, k odd or even
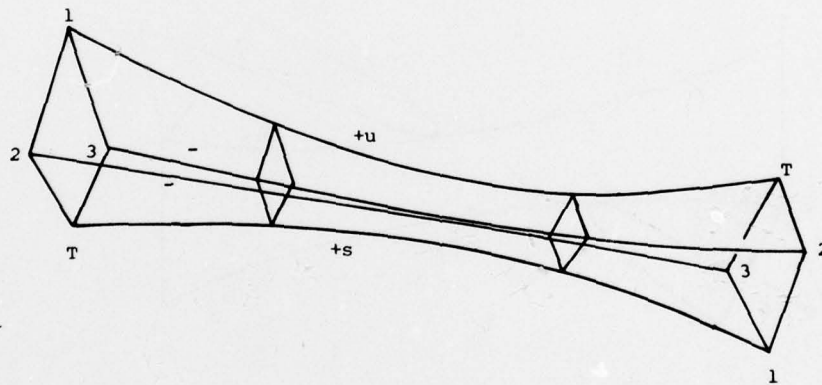
Figure 2.4d$_2$: III$_1$, $\varepsilon > 0$, region 1, k odd or even

-24-
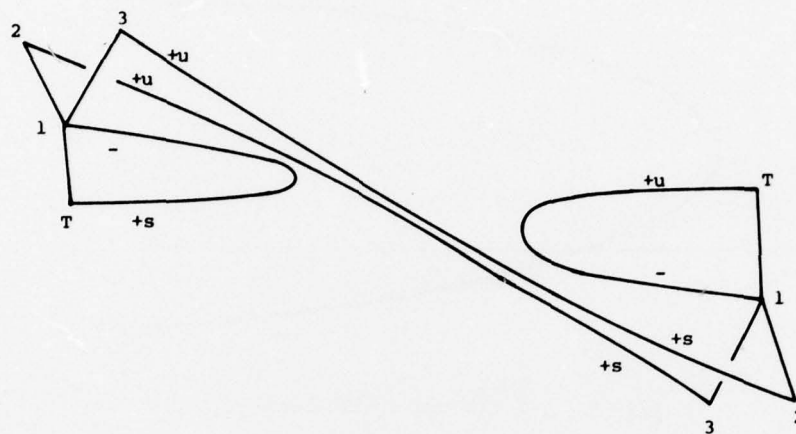
Figure 2.4e$_1$: III$_2$, $\varepsilon > 0$, k odd
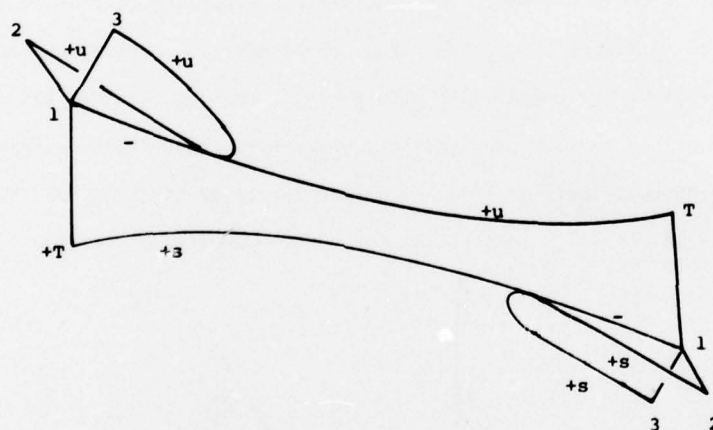
Figure 2.4e$_2$: III$_2$, $\varepsilon > 0$, k even

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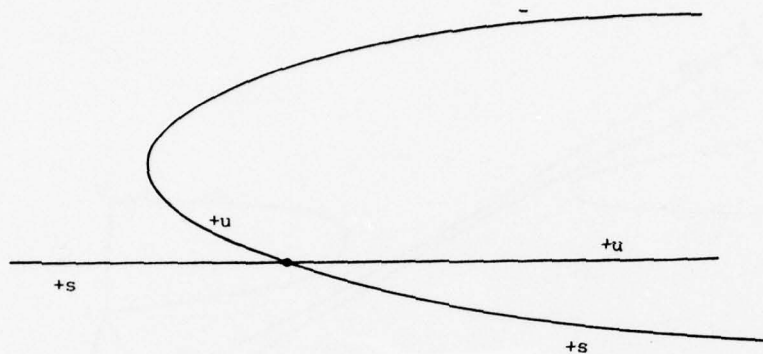
Figure 2.5: Behavior in the large

must be regarded as the generic cases, since points (δ, ε) whose components are of the same order will belong to these regions. The diagrams corresponding to regions 3 and 6 are those illustrated in Figures $2.4c_1$ and $2.4c_2$, respectively; the diagrams corresponding to the four thin regions are required to effect the transition between regions 3 and 6. It is quite possible to imagine situations where these transition diagrams are relevant, but we suspect that their detailed structure is too specialized for the model at hand. We refer the interested reader to [3] for a more complete discussion.
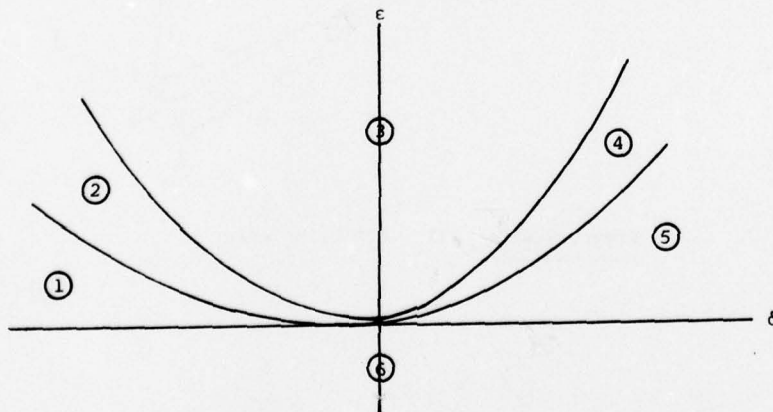
Figure 2.6

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§3. Review of the classification results of [ ]

In the next section we will apply the Lyapunov-Schmidt reduction to the equilibrium equation (1.14) and will obtain a system of the form

$$(3.1) \quad \begin{cases} a_1 x^2 + a_2 y^2 + b_1 \lambda x = 0 \\ \qquad\quad a_3 xy + b_2 \lambda y = 0 \;, \end{cases}$$

at least modulo cubic terms. These equations represent the most general reduced equations at a double eigenvalue for a system governed by a quadratic non-linearity and possessing the symmetry

$$(3.2) \qquad\qquad\qquad J\underline{G}(J\underline{x},\lambda) = \underline{G}(\underline{x},\lambda) \;,$$

where J is the matrix

$$J = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

In this section we recall some of the definitions and results of [3] concerning the classification of such problems.

Let $G, H : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$ be two reduced bifurcation problems, defined near the origin. We shall call G and H <u>contact equivalent</u> if there exists an invertible, 2×2 matrix-valued function $\tau_{x,\lambda}$ and a diffeomorphism on $\mathbb{R}^2 \times \mathbb{R}$ of the form $(x,\lambda) \mapsto (\rho(x,\lambda),\Lambda(\lambda))$ such that

$$(3.3) \qquad\qquad H(x,\lambda) = \tau_{x\lambda} \cdot G(\rho(x,\lambda),\Lambda(\lambda)) \;.$$

We are primarily interested in bifurcation diagrams such as (1.17), and it is clear that the bifurcation diagram of G is not changed at all by multiplication by an invertible matrix. The diffeomorphism (ρ,Λ) represents only an inessential change of coordinates in the problem, which will not change the qualitative nature of the bifurcation diagram. These remarks are intended to motivate our definition. (In general transformations such as (3.3) <u>can</u> change the stability assignments of the various solution branches in a bifurcation diagram. However the degree of a solution branch is well defined since we require that $\tau_{x\lambda}$ and $d\rho$, the differential of ρ, have positive determinants. We ignore the stability issue for the time being, returning to it in §7.)

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The above definition neglects the symmetry of (3.1). The appropriate coordinate transformations (ρ, Λ) which preserve symmetry must satisfy (3.2) and the matrices $\tau_{x\lambda}$ must satisfy

$$(3.4) \qquad\qquad J^{-1} \tau_{Jx,\lambda} J = \tau_{x\lambda} \ .$$

(In practice (3.4) simply means that the diagonal entries of τ are *even functions* of y; the off diagonal entries, odd.) We shall call two problems G and H <u>equivariantly</u> <u>contact</u> <u>equivalent</u> if (3.3) is satisfied and all functions have the appropriate symmetry. Usually we abbreviate this phrase to <u>equivalent</u>.

It is shown in [3] that the classification of problems of the form (3.1), up to equivalence, depends only on

$$(3.5) \qquad\qquad c = \frac{b_1 a_3}{b_2 a_1} \ \text{ and } \ \eta = \text{sign}(a_1 a_2) \ .$$

In other words (3.1) is equivalent to (1.16), where c and η are given by (3.5). The type of the bifurcation diagram as a function of the parameters c and η is given in Figure 3.1. Strictly speaking any two problems of the form (1.16) with different

	$c < 0$	$0 < c < 1$	$c > 1$
$\eta = +1$	I_0	I_0	III_1
$\eta = -1$	III_0	III_2	I_1

Figure 3.1

values of c are inequivalent, but in practice the qualitative features of the bifurcation diagram are unchanged if c remains within one of the intervals of Figure 3.1. Moreover, provided c avoids the boundaries of these intervals, the higher order terms that were neglected in writing (3.1) may in fact be transformed away by an auspicious choice of τ, ρ, Λ.

Reference [3] also considers perturbations of (3.1), in terms of the following specific definition. By an <u>unfolding</u> of a bifurcation problem $G : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$ we mean a

smooth map $F : \mathbb{R}^2 \times \mathbb{R} \times \mathbb{R}^\ell \to \mathbb{R}^2$ such that $F(\mathbf{x},\lambda,0) = G(\mathbf{x},\lambda)$. The ℓ variables in the third argument of F will be called unfolding parameters. We show in [3] that

$$(3.6) \qquad \underline{F}(\underline{x},\lambda,\alpha,\beta,\gamma) = \begin{pmatrix} x^2 + \eta y^2 + \lambda x + \alpha \\ (c + \gamma)xy + (\lambda + \beta)y \end{pmatrix}$$

is a universal unfolding of (1.16) relative to equivalence, assuming $c \neq 0,1$. This means in particular that given an unfolding of (1.16) of the form $F(\cdot,\cdot,\varepsilon) = G + \varepsilon H$, there exist smooth functions $\alpha(\varepsilon)$, $\beta(\varepsilon)$, $\gamma(\varepsilon)$, defined for small ε, such that $G_0 + \varepsilon H$ is equivalent to $F(\cdot,\cdot,\alpha(\varepsilon),\beta(\varepsilon),\gamma(\varepsilon))$. See [3] for a more thorough discussion of these issues.

The reader will note that our universal unfolding (3.6) contains three unfolding parameters, while we indicated above that two parameters suffice to describe perturbations of (1.16). The explanation of this discrepancy is as follows. The parameter c determines the overall character of the bifurcation, but, as noted above, once it is restricted to one of the intervals in Figure 3.1, small changes in this parameter do not affect the qualitative nature of the bifurcation. Thus we regard γ as an inessential parameter for our present purposes.

The following table indicates the correspondence between the notation of the present paper and that of [3] in naming the various cases which arise.

Present notation	I_0	I_1	III_0	III_1	III_2
Notation of [3]	2h	2e	$4e_0$	4h	$4e_\infty$

Figure 3.2

§4. The Lyapunov-Schmidt reduction for the unperturbed case

Let us begin our discussion with some comments about the interpretation of (1.4) and its associated equilibrium equation (1.14). We consider (1.4) as an evolution equation on the Banach space $X = C^0([0,\pi], \mathbb{R}^2)$. We could of course regard L as an unbounded linear operator on X with domain

$$D = \{w \in C^2([0,\pi], \mathbb{R}^2) : w(0) = w(\pi) = 0\} ,$$

but we prefer to regard L as a bounded linear operator $L : D \to X$, where D has the C^2 topology. Moreover N, considered as a map from D into X, is C^∞ Fréchet differentiable - indeed N is already smooth considered as a map from X into itself. Thus the right hand side of (1.4), namely $L + N$, defines a C^∞ mapping $\Phi : D \to X$. Note that $(d\Phi)_0 = L$, which is a Fredholm operator of index zero.

Let $X_0 = \ker L$ and $X_1 = \text{range } L$. We shall assume below that X admits the decomposition

(4.1)
$$X = X_0 \oplus X_1 .$$

This means that all the generalized eigenfunctions of L associated to the eigenvalue zero already belong to $\ker L$; in other words, $\ker L^2 = \ker L$. We also suppose that the spectrum of L restricted to X_1 is properly contained in the stable half plane, say

(4.2)
$$\sigma(L|X_1) \subset \{\zeta : \text{Re}\,\zeta \le -\varepsilon\}$$

where $\varepsilon > 0$. Since $X_0 \subset D$, it follows that $D = X_0 \oplus D_1$, where $D_1 = D \cap X_1$. Also, $L : D_1 \to X_1$ is a linear isomorphism between the two Banach spaces. Let E_0, E_1 be the projections associated to the decomposition (4.1).

In the Lyapunov-Schmidt reduction one eliminates all but a finite number of components of w in (1.14) by inverting the non-singular part of L. Specifically define a mapping $W : X_0 \to D_1$ implicitly by

(4.3)
$$E_1 \Phi(x + W(x)) = 0$$

for $x \in X_0$. It follows from the implicit function theorem that (4.3) is soluble in some neighborhood of zero. Let $G : X_0 \to X_0$ be defined by

(4.4)
$$G(x) = E_0 \Phi(x + W(x)) .$$

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Then $x + W(x)$ is a solution of (1.14) if and only if $G(x) = 0$, and every solution of (1.14) has this form.

For computations it is convenient to have a reformulation using coordinates of the Lyapunov-Schmidt reduction, carrying explicitly the bifurcation parameter λ . Let w_1 , w_2 be a basis for χ_0 . If we parametrize χ_0 by $\mathbb{R}^2$ via the map $\underline{x} \to xw_1 + yw_2$, then we may rewrite (4.3) as

(4.5) $$LW(\underline{x},\lambda) + E_1 N(xw_1 + yw_2 + W(\underline{x},\lambda)) = 0 .$$

Let w_1^* , w_2^* be a basis for $\ker L^*$, where L^* is the adjoint of L , normalized so that

(4.6) $$\langle w_i^*, w_j \rangle = \alpha \delta_{ij}$$

for some positive constant α . (Here and below $\langle \cdot, \cdot \rangle$ denotes the L^2 inner product.) Then, in terms of the coordinates on χ_0 above, E_0 has the representation

(4.7) $$E_0 w = (\langle w_1^*, w \rangle, \langle w_2^*, w \rangle) .$$

Thus equation (4.4), defining the reduced mapping $\underline{G} : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$, may be rewritten in components as

(4.8) $$G_i(\underline{x},\lambda) = \langle w_i^*, \Phi(xw_1 + yw_2 + W(\underline{x},\lambda)) \rangle ,$$

where $i = 1,2$. We shall always take w_1 to be even with respect to (1.13) and w_2 odd; w_1^* and w_2^* inherit the corresponding parities by (4.6).

We may perhaps avoid confusion if we introduce notation to indicate the dependence on B that is implicit in L . Let us write $L = L_0 + \lambda M$, where L_0 is given by (1.5), with B fixed at the bifurcation point, and

(4.9) $$Mw = u \begin{pmatrix} 1 \\ -1 \end{pmatrix} .$$

Using the fact that $L_0^* w_i^* = 0$ we may rewrite (4.8) as

(4.10) $$\underline{G}_i(\underline{x},\lambda) = \langle w_i^*, (\lambda M + N)(xw_1 + yw_2 + W(\underline{x},\lambda)) \rangle .$$

We now start the computation of the coefficients in (3.1) as functions of the various parameters in our problem. In the following lemma $d^2 N$ denotes the second Fréchet derivative of N , a bilinear mapping $X \times X \to X$.

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Lemma 4.1: The second order derivatives of the reduced map $\underline{G}$ at the origin are given by

$$\frac{\partial^2 G_i}{\partial x_j \partial x_\ell} = (w_i^*, d^2 N(w_j, w_\ell))$$

$$\frac{\partial^2 G_i}{\partial x_j \partial \lambda} = (w_i^*, M w_j) \; .$$

Proof: It follows by differentiation of (4.10) that (when $\lambda = 0$)

$$(4.11) \qquad \frac{\partial^2 G_i}{\partial x_j \partial x_\ell} = (w_i^*, d^2 N(w_j + \frac{\partial W}{\partial x_j}, \; w_\ell + \frac{\partial W}{\partial x_\ell})) \; + (w_i^*, dN \cdot \frac{\partial^2 W}{\partial x_j \partial x_\ell}) \; .$$

However dN is zero at the origin. This means that the second term in (4.11) vanishes at the origin and that, by (4.5), $\frac{\partial W}{\partial x_j}$ also vanishes there. This verifies the first formula in the lemma, and the argument for the second is similar. The proof is complete.

We do not reproduce the details of the computation of the coefficients in (3.1), but only record the landmarks as a guide to the reader. It follows from (1.6) that at the origin

$$(4.12) \qquad d^2 N(w_1, w_2) = 2\{\frac{B}{A} u_1 u_2 + A(u_1 v_2 + v_1 u_2)\} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \; .$$

The eigenfunctions of L and L^* at the double eigenvalue are given by

$$(4.13) \qquad \left\{ \begin{array}{ll} w_1(\xi) = \sin k\xi \begin{pmatrix} \theta D\mu_1 \\ -1 - D\mu_1 \end{pmatrix} & w_2(\xi) = \sin(k+1)\xi \begin{pmatrix} \theta D\mu_2 \\ -1 - D\mu_2 \end{pmatrix} \\[20pt] w_1^*(\xi) = \sin k\xi \begin{pmatrix} 1 + D\mu_2 \\ D\mu_2 \end{pmatrix} & w_2^*(\xi) = f_1 \sin(k+1)\xi \begin{pmatrix} 1 + D\mu_1 \\ D\mu_1 \end{pmatrix} \end{array} \right. ,$$

where

$$(4.14) \qquad f_1 = \frac{\theta\mu_1 - \mu_2 + D\mu_1\mu_2(\theta - 1)}{\theta\mu_2 - \mu_1 + D\mu_1\mu_2(\theta - 1)}$$

is a correction factor required by the normalization (4.6). The reader will note that if k is odd, then w_1 in (4.13) is even with respect to the symmetry (1.13). Suppose

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that the two wave numbers at the double eigenvalue are ℓ and $\ell + 1$. If ℓ is odd, we shall use (4.13) with $k = \ell$; if ℓ is even, we shall use (4.13) with $k = -(\ell + 1)$. By this ruse we can always arrange that the smaller wave number (in the algebraic sense) at the double eigenvalue is odd. In this way we may observe the parity convention introduced above and still avoid carrying two sets of formulas for the eigenfunctions.

On substitution of (4.9), (4.12), and (4.13) into the formulas of Lemma 4.1, one finds after appropriate manipulation, the following formulas for the coefficients in (3.1).

(4.15a)
$$a_1 = \left\{ \frac{\mu_1}{\mu_2} - 2\,\frac{D\mu_1}{1 + D\mu_2} \right\} I_1$$

(4.15b)
$$a_2 = \left\{ \frac{\mu_2}{\mu_1} - 2\,\frac{D\mu_2}{1 + D\mu_1} \right\} I_2$$

(4.15c)
$$a_3 = 2f_1 \left\{ 1 - \frac{D\mu_1}{1 + D\mu_1} - \frac{D\mu_2}{1 + D\mu_2} \right\} I_2$$

(4.15d)
$$b_1 = \frac{\pi}{2}\,\theta D\mu_1$$

(4.15e)
$$b_2 = f_1\,\frac{\pi}{2}\,\theta D\mu_2 .$$

Here we have used the notation

$$I_1 = \theta AB \int_0^\pi \sin^3 k\xi\, d\xi$$

$$I_2 = \theta AB \int_0^\pi \sin k\xi\, \sin^2(k+1)\xi\, d\xi .$$

Note that I_1, I_2 have the same sign as k.

According to the results of [3] quoted in §3 of the present paper, the qualitative type of the bifurcation diagram associated to (3.1) can change only if one of the following equations is satisfied.

(4.16)
$$\begin{cases} \text{(a)} \quad a_1 = 0 \qquad\qquad \text{(b)} \quad a_2 = 0 \\ \text{(c)} \quad a_3 = 0 \qquad\qquad \text{(d)} \quad b_1 a_3 = b_2 a_1 \end{cases}$$

Let us consider the simplest of these equations, (4.16c). On multiplying (4.15c) by

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$(1 + D\mu_1)(1 + D\mu_2)$ and dividing by a non-zero factor we may rewrite (4.16c) as

$$1 - D^2\mu_1\mu_2 = 0 \ .$$

We may combine the definitions of §1 to show that $\bar{A}^2 = D^2\mu_1\mu_2$, from which it follows that (4.16c) is satisfied if and only if $\bar{A} = 1$. The reader will note that this line appears as one of the dividing curves in Figure 2.1, both cases (a) and (b).

Consideration of equations (4.16a) and (4.16b) is similar. First invoke (4.15) to show that these equations are satisfied if and only if

(4.17) (a) $D\mu_2 = 1$ (b) $D\mu_1 = 1$

respectively, and then use the definitions of §1 to express (4.17) in terms of the parameters $\bar{A}$ and D. If k is positive, the result is that (4.16a or b) is satisfied if and only if

(4.18) (a) $D = (\bar{A} - 1)^2$, $\bar{A} < 1$

(b) $D = (\bar{A} - 1)^2$, $\bar{A} > 1$

respectively; if k is negative, the formula $D = (\bar{A} - 1)^2$ remains valid but the inequalities in (4.18) are reversed. The reader will again note that the parabola $D = (\bar{A} - 1)^2$ occurs as a dividing curve in Figure 2.1. The remaining, unidentified dividing curve in the figures is of course associated with (4.16d). Its equation may be written

(4.19) $2f_2(1 - D^2\mu_1\mu_2) - (1 + D\mu_1)(1 - D\mu_2) = 0$,

where

$$f_2 = I_2/I_1 = \frac{3(k + 1)^2}{(k + 2)(3k + 2)} \ ,$$

but (4.19) does not seem to admit a simple representation as a function of $\bar{A}$ and D.

In Figure 4.1 we have tabulated the signs of the coefficients (4.15) in the various regions using the notation (3.5). The type of the bifurcation diagram may be determined by comparison with Figure 3.1.

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Region number	a_1	a_2	a_3	c	$c - 1$	η	Type of diagram
1	+	+	+	+	+	+	III_1
2	−	+	+	−	−	−	III_0
3	−	+	−	+	−	−	III_2
4	−	−	−	+	−	+	I_0
5	−	−	−	+	+	+	III_1

Figure 4.1a: k positive

Region number	a_1	a_2	a_3	c	$c - 1$	η	Type of diagram
1	−	−	−	+	+	+	III_1
2	−	+	−	+	+	−	I_1
3	−	+	−	+	−	−	III_2
4	−	+	+	−	−	−	III_0
5	+	+	+	+	+	+	III_1

Figure 4.1b: k negative

§5. Lyapunov-Schmidt calculations for the perturbed problems

It may perhaps give a clearer exposition if we indicate how to compute the unfolding parameters in (3.6) for a general perturbation of the equilibrium equation (1.14), although for the problem at hand we are able to avoid the most unpleasant aspects of this calculation. Suppose (1.14) is modified by a perturbation term to read

$$(5.1) \qquad\qquad \Phi(w) + \varepsilon P(w) = 0 .$$

Let E_0, E_1 be defined as in §4 to be the projections relative to the decomposition (4.1), this data being computed only for $\varepsilon = 0$. We define the reduced equations, depending on ε, as follows. Let $W : \mathcal{X}_0 \times \mathbb{R} \to D_1$ be defined implicitly by

$$(5.2) \qquad\qquad E_1(\Phi + \varepsilon P)(x + W(x,\varepsilon)) = 0$$

and let

$$(5.3) \qquad\qquad G(x,\varepsilon) = E_0(\Phi + \varepsilon P)(x + W(x,\varepsilon)) .$$

Translation of these expressions into coordinate notation poses no special difficulties, although it should be mentioned that, unlike in §4, the function W plays a role here. It follows from the natural analogue of (4.5) that at the origin

$$(5.4) \qquad\qquad \frac{\partial W}{\partial \varepsilon} = -L^{-1} E_1 P ,$$

where L^{-1} is the generalized inverse of L. Suppose we define coefficients for the perturbed problem by

$$G_i(x,\varepsilon) - G_i(x,0) = \varepsilon\{\alpha_i + \sum_{j=1}^{2} \beta_{ij} x_j + \beta_{i0}\lambda\} + \text{hot} ,$$

where the higher order terms include terms of order ε^2, εx^2, $\varepsilon\lambda^2$. A straightforward calculation shows that

$$(5.5a) \qquad\qquad \alpha_i = \langle w_i^*, P \rangle$$

$$(5.5b) \qquad\qquad \beta_{ij} = \langle w_i^*, dP(w_j) - d^2 N(L^{-1} E_1 P, w_j) \rangle$$

$$(5.5c) \qquad\qquad \beta_{i0} = \langle w_i^*, \frac{\partial P}{\partial \lambda} - M L^{-1} E_1 P \rangle .$$

The only significant difference between these formulas and those of Lemma 4.1 is the appearance of a second term in the inner products of (5.5b and c), and this difference is a direct consequence of (5.4).

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Let us first compute the unfolding parameters for the perturbation associated
to (1.12). It is readily seen that

$$A(\xi) = A_0 - \frac{\varepsilon A_0}{2} \xi(\pi - \xi) + O(\varepsilon^2) .$$

Note that A appears only in the first equation of (1.1), and there only additively.
(Remark: In the passage to (1.4) we still linearize about a constant function,
namely $X = A_0$, $Y = B/A_0$.) Thus in the notation of (5.1) we should define

$$(5.6) \qquad\qquad P = - \frac{1}{2} A_0 \xi(\pi - \xi) \begin{pmatrix} 1 \\ 0 \end{pmatrix} ,$$

a perturbation which is independent of w. We compute from (5.5a) that $\alpha_2 = 0$, as
required by symmetry, and that

$$(5.7) \qquad\qquad \alpha_1 = - \frac{2A_0}{k^3} (1 + D\mu_2) .$$

The computation of the first order terms β_{ij} would be rather tedious because of the
presence of L^{-1} in the relevant formulas. However, we recall from §3 that the
zeroth order coefficient α in (3.6) dominates the first order coefficient β, provided
they are of the same order, which is the case here, since (5.7) shows that α is non-
vanishing. Thus the effect of the perturbation (5.6) is determined by the sign of α
(negative) and the sign of the coefficients in Figure 4.1. The reader may consult [3]
to check the validity of the diagrams of Figure 2.4.

The perturbation associated to changes in the diffusion coefficient D admits the
representation

$$(5.8) \qquad\qquad Pw = \begin{pmatrix} 1 & 0 \\ 0 & \theta \end{pmatrix} \frac{\partial^2 w}{\partial \xi^2} ,$$

which depends linearly on w. We could easily substitute (5.8) into (5.5) and evaluate
the resulting expressions – this perturbation differs from the preceding one in that
here P vanishes at the origin, eliminating the troublesome terms with L^{-1}. However,
there is a direct way to assess the effect of (5.8), which moreover sheds some insight
on the problem. This perturbation splits apart the double eigenvalue but does not

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affect the existence of the trivial solution. We may see from (3.6) that there is essentially only one way to do this, namely to change β but to keep α equal to zero. Thus to describe the perturbed diagram we need only know which mode bifurcates from the trivial solution first, and we can decide this by an independent argument.

Let us recall (1.9), the formula for the bifurcation point of the mode with wave number ℓ from the trivial solution

$$(5.9) \qquad B_\ell = 1 + \frac{A^2}{\partial} + D\ell^2 + \frac{A^2}{\theta D\ell^2} .$$

Observe that we may write (5.9) as a function of a real variable $D\ell^2$, say $B_\ell = f(D\ell^2)$. By hypothesis

$$\min_\ell \{f(D\ell^2): \quad \ell = 1,2,3,\ldots\}$$

is assumed at two distinct integers k and $k + 1$, as indicated in Figure 5.1. It may be seen by inspection that increasing D lowers B_k and raises B_{k+1}. In other words, increasing D makes the mode with smaller wave number (in absolute value) bifurcate first. This is the behavior portrayed in Figure 2.2. To facilitate the reader's checking this statement, we mention that the solution points of the mode with odd wave number are located in the plane of symmetry of the bifurcation diagram, while those with even wave number occur in symmetric pairs.
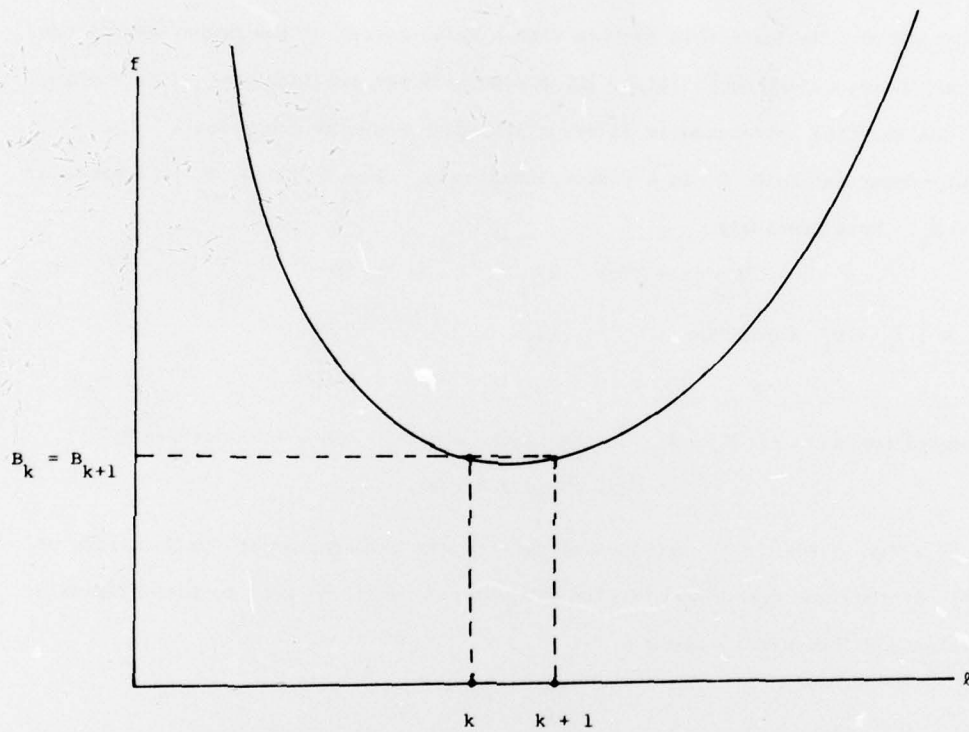
Figure 5.1

§6. On the relation between the Lyapunov-Schmidt and center manifold reductions

The Lyapunov-Schmidt reduction enumerates all rest points of (1.4) but provides no information about the dynamical behavior of this equation. In this respect reduction of (1.4) via the center manifold theorem is preferable, although somewhat less straightforward. We begin this section with a brief review of the properties of the center manifold, referring to [4] or [8] for details not provided below. We continue to use the notation introduced in §4 for the Lyapunov-Schmidt reduction.

The center manifold M is a finite dimensional submanifold of X parametrized by $x \in X_0$. More precisely

(6.1) $$M = \{x + V(x) : x \in X_0 \text{ close to zero}\}$$

where $V : X_0 \rightarrow D_1$ satisfies

(6.2) $$(E_1 - dV \cdot E_0) \Phi(x + V(x)) = 0 .$$

The reduced mapping $H : X_0 \rightarrow X_0$ in the center manifold context is defined by

(6.3) $$H(x) = E_0 \Phi(x + V(x)) .$$

Thus $\{x + V(x) : H(x) = 0\}$ provides an alternative enumeration of the solutions of (1.14). At the same time, however, the trajectories of (1.4) tend to trajectories of the ordinary differential equation

(6.4) $$\frac{dx}{dt} = H(x)$$

in the following sense. Let U be an appropriately small neighborhood of zero in X, let $w(t)$ be a solution of (1.4) such that $w(t) \in U$ for $0 \leq t \leq T$, and let

$$\delta(t) = \| E_1 w(t) - V(E_0 w(t)) \| ,$$

the distance between $w(t)$ and its projection into M. Then

$$\delta(t) \leq C e^{-\varepsilon t/2} \delta(0)$$

for $0 \leq t \leq T$, where ε is defined by (4.2). The constant C depends only on U in the above data. Unfortunately this result does not state in general to what extent the projection $x(t) = E_0 w(t)$ is approximated by a solution of (6.4), but if $\delta(0) = 0$

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(i.e., if $w(0) \in M$), then $x(t)$ is actually a solution of (6.4). Moreover if $S \subset X_0$ is an attracting set for (6.4), then $\{x + V(x) : x \in S\}$ is attracting for (1.4).

Equation (6.2) expresses the condition that the flow direction $\Phi(w)$ be tangent to M when $w \in M$. To see this let us define a smooth mapping $f : X \to X_1$ by

$$f(w) = E_1 w - V(E_0 w) ,$$

so that $M = f^{-1}(0)$. We may write the condition of tangency as

$$\frac{d}{dt} f(w(t)) = 0 .$$

Since M is contained in D, $\frac{dw}{dt}$ is well defined for $w \in M$. Application of the chain rule leads to (6.2).

In one sense (6.2) is a small perturbation of (4.3); namely, since dV, Φ, and $E_0 \cdot d\Phi$ all vanish at the origin the perturbing term may be expected to be small near zero. On the other hand the new term in (6.2) involves derivatives of V, which makes an existence proof for (6.2) by a direct perturbation argument problematic. Indeed this existence question is discussed in [4] in terms of the non-linear semigroup of transformations generated by Φ. Moreover because of the singular nature of this perturbation, (6.2) does not necessarily admit C^∞ solutions. Although there are C^k solutions for arbitrarily large k, the size of the domain of existence decreases as k increases. However, the fact that dV, Φ, and $E_0 \cdot d\Phi$ all vanish at the origin does have the following consequence: in computing derivatives of V at the origin from (6.2), the second term will always contribute to lower order than the first. Thus for example

(6.5) $$\frac{\partial^2 V}{\partial x_i \partial x_j} = -L^{-1} d^2 \Phi(e_i, e_j)$$

where $L^{-1} : X_1 \to D_1$ is a pseudo-inverse and $\{e_i\}$ is a basis for X_0; the same formula holds for $\partial^2 W / \partial x_i \partial x_j$.

There is a minor technical issue to be addressed before the results of [4] are formally applicable. We must modify (1.4) outside of a neighborhood of zero in order to verify the hypotheses of [4]. Let χ be a C^∞ function with compact support on

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the finite dimensional space X_0, $\chi \equiv 1$ near zero. We modify (1.4) to read

$$\frac{\partial w}{\partial t} = L(w) + \chi(E_0 w)N(w) ,$$

so that the equation is linear when $E_0 w$ is large. It is then a simple matter to verify the estimates needed in [4] to construct the center manifold. For this verification the reader should note the following fact: $N(w)$ vanishes to second order, so by restricting the support of χ we may arrange that χN and its first derivatives are as small as may be necessary. Also if Φ depends smoothly on a finite number of parameters, it is shown in [4] that the center manifold depends C^k-smoothly on those parameters.

The fact that the center manifold is only finitely differentiable would lead to certain technical complications if we attempted to apply the center manifold theorem directly. The following lemma provides a relation between the center manifold and the Lyapunov-Schmidt reductions that may be exploited to avoid these complications. The matrix σ_x in the lemma depends on the parameters B, A, D_i in the problem but we do not indicate this dependence explicitly.

Lemma 6.1: There exists a C^k matrix-valued function σ_x such that the reduced mappings G and H of formulas (4.4) and (6.3) are related by

(6.6) $$H(x) = \sigma_x \cdot G(x).$$

Moreover σ_x is invertible and $\sigma_x = I + O(x^2)$.

Proof: As a technical device we introduce additional parameters into the arguments of G and H. Let us define an extended function $\tilde{\Phi} : D \times X_0 \to X$ by

$$\tilde{\Phi}(w,y) = \Phi(w) + y .$$

We redefine all the functions above to include these extra parameters, indicating the change with a twiddle. Thus for example $\tilde{v} : X_0 \times X_0 \to X_1$ is defined by

(6.7) $$(E_1 - d_x \tilde{v} \cdot E_0)\Phi(x + \tilde{v}(x,y)) - d_x \tilde{v} \cdot y = 0 ,$$

where we have used the relation $E_1 y = 0$ to discard a term. It turns out that

(6.8) $$\tilde{G}(x,y) = G(x) + y .$$

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It is clear from this equation that

(6.9) $\{(x,y) : \tilde{G}(x,y) = 0\}$

is a smooth submanifold of $X_0 \times X_0$, which is the reason for introducing the additional parameters.

The fundamental observation in this proof is that $\tilde{G}(x,y) = 0$ if and only if $\tilde{H}(x,y) = 0$ - both reductions yield all rest points of the equation. Therefore each component of $\tilde{H}(x,y)$ vanishes on the smooth manifold (6.9), so by Taylor's theorem each such component may be written as a linear combination (with variable coefficients) of the functions defining (6.9), namely the components of $\tilde{G}$ itself. In other words we have

(6.10) $\tilde{H}(x,y) = \sigma_{xy}\tilde{G}(x,y)$

for some matrix-valued function σ. We obtain (6.6) on restricting (6.10) to $y = 0$. The proof that $\sigma_x = I + O(x^2)$ is based on the computation of various derivatives of (6.10) indicated below. Given this, it follows that σ_x is invertible for small x.

The derivatives we shall need first are

(6.11) $\dfrac{\partial \tilde{G}}{\partial x_i} = 0, \quad d_y \tilde{G} = I, \quad \dfrac{\partial^2 \tilde{G}}{\partial x_i \partial y_j} = 0$

for $x = y = 0$. The last two relations are obvious, in view of (6.8), and the first follows from (4.4) on observing that

(6.12) $E_0 \cdot d\Phi = 0$.

We claim that $\tilde{H}$ satisfies the same relations (6.11). Now

(6.13) $\tilde{H}(x,y) = E_0 \Phi(x + \tilde{v}(x,y)) + y$.

The first two relations in (6.11) follow immediately from (6.13) by differentiation, if (6.12) is recalled. As to the third relation in (6.11), we have

(6.14) $\dfrac{\partial^2 \tilde{H}}{\partial x_i \partial y_j} = E_0 d^2\Phi(e_i + \dfrac{\partial \tilde{v}}{\partial x_i}, \dfrac{\partial \tilde{v}}{\partial y_j})$,

again making use of (6.12) to drop a term. We argue that $\partial\tilde{v}/\partial y_j = 0$ as follows. Differentiate (6.7) with respect to x_i and evaluate at $x = y = 0$. This yields simply

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(6.15) $$E_1 \cdot d\Phi \cdot \frac{\partial \tilde{V}}{\partial x_i} = 0 \; ;$$

the terms involving $d\tilde{V} \cdot E_0 \cdot \Phi$ and $d\tilde{V} \cdot y$ do not contribute to (6.15) because of
(6.12) and because $y = 0$, respectively. But $E_1 \cdot d\Phi = L$ is one-to-one on D_1,
the space to which $\tilde{V}$ belongs, so $\partial \tilde{V}/\partial x_i = 0$. Similarly differentiation of (6.7)
with respect to y_j leads to the conclusion $\partial \tilde{V}/\partial y_j = 0$; in this case (6.15) may be
used to drop the last term of (6.7). This proves the claim above.

On differentiating (6.10) with respect to y and evaluating at $x = y = 0$ we
find that

$$d_y \tilde{H} = \sigma_{xy} \cdot d\tilde{G} \; ,$$

where we have discarded a term containing $\tilde{G}(0,0)$, which vanishes. It follows from
(6.11) that $\sigma_{xy} = I$ when $x = y = 0$. Taking mixed second derivatives of (6.10) yields
the relation

$$0 = \frac{\partial \sigma}{\partial x_i} \cdot d\tilde{G} \; ;$$

here we have used (6.11) to discard one term on the left and three on the right. There-
fore $\partial \sigma/\partial x_i = 0$ at the origin, and the proof is complete.

Of course when the center manifold reduction is implemented for (1.4) in the
coordinates on X_0 introduced in §4, the reduced mapping H will possess the symmetry
(3.2) and the matrix σ_x of Lemma 6.1 will satisfy (3.4).

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§7. Stability of the bifurcating solutions

The goal of the present section is to verify the stability assignments made in drawing the bifurcation diagrams of §2. We do this by ad hoc arguments which depend strongly on the symmetry (1.13).

The bifurcation diagram

$$(7.1) \qquad \{(x,\lambda) : H(x,\lambda) = 0\}$$

enumerates the equilibrium solutions of (1.4). Here H is the reduced mapping on the center manifold, as defined by (6.3). In the discussion below we suppress the dependence of H on all external parameters, including the bifurcation parameter λ. According to §6 the stability or instability of any equilibrium solution of (1.4) enumerated by (7.1) is determined by the stability or instability of the corresponding rest point of the ordinary differential equation (6.4). However by Lemma 6.1 we may express H in terms of G, the reduced mapping of the Lyapunov-Schmidt reduction, and G in turn may be expressed in terms of the universal unfolding (3.6),

$$(7.2) \qquad G = \tau_x F \circ \rho \ .$$

On combining these observations we see that (6.4) may be written

$$\frac{dx}{dt} = \sigma_x \tau_x F \circ \rho(x) \ .$$

If we introduce the change of coordinates $x' = \rho(x)$, we may compute that

$$(7.3) \qquad \frac{dx'}{dt} = \bar{\tau}_x F(x') \ ,$$

where $\bar{\tau}_x = d\rho \cdot \sigma_x \cdot \tau_x$. To summarize, we saw in §3 that the rest points of (1.4) may be enumerated by the zeros of F; here we see that the stability properties of these rest points may also be obtained from F through analysis of (7.3).

The stability or instability of rest points of (7.3) is of course determined by the real parts of the eigenvalues of the Jacobian of this equation, which at a rest point of (7.3) equals $\bar{\tau}_x dF$. But the stability assignments on the bifurcation diagrams in §2 were made by an inspection of the eigenvalues of dF, or in other words, were made according to the stability of

$$(7.4) \qquad \frac{dx}{dt} = F(x) \ .$$

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Thus our task in the present section is to show that the real parts of the eigenvalues of dF are not changed by multiplication by $\bar{\tau}_x$.

The basic fact we will use in this derivation is that $\bar{\tau}_x$ satisfies (3.4), which follows from the fact that each of the factors in the definition of $\bar{\tau}_x$ satisfies (3.4). Thus in the plane of symmetry (i.e., when $y = 0$), $\bar{\tau}_x$ is diagonal. We claim in fact that the diagonal entries of $\bar{\tau}_x$ are both positive in this plane. It suffices to look at the origin, since τ_x is non-singular and cannot have a vanishing diagonal entry. At the origin $\sigma_x = I$ and may be ignored. Taking an appropriate mixed derivative of (7.2) we find that at the origin

$$d\left(\frac{\partial G}{\partial \lambda}\right) = \tau_x \cdot d\left(\frac{\partial F}{\partial \lambda}\right) \cdot d\rho \; ;$$

only one non-zero term results from differentiation on the right since F vanishes to second order. However it may be seen from (3.6) that $d\left(\frac{\partial F}{\partial \lambda}\right) = I$, and $d\left(\frac{\partial G}{\partial \lambda}\right)$ is a diagonal matrix with entries b_1, b_2 given by (4.15), both positive. Thus the diagonal entries of the product $\tau_x \cdot d\rho$ are positive at the origin, and being diagonal, these matrices commute. This proves the above claim. In the following we shall omit the bar in $\bar{\tau}_x$, as we have no further occasion to refer to the individual factors in this matrix.

If the parameters c and η in (3.6) have the same sign, we claim that (7.3) and (7.4) admit a common Lyapunov function, and hence have the same stability properties. The Lyapunov function is

$$(7.5) \qquad \phi(x,y) = \frac{x^3}{3} + \eta x y^2 + \lambda \frac{x^2}{2} + \frac{\eta(\lambda + \beta)}{c'} y^2 + \alpha x \; ,$$

where $c' = c + \gamma$. We suppose that γ is small so that c' and η also have the same sign. To check that (7.5) is a Lyapunov function for (7.4), we compute that

$$(7.6) \qquad \langle F, \text{grad } \phi \rangle = (x^2 + \eta y^2 + \lambda x + \alpha)^2 + \frac{2\eta}{c'}(c'xy + (\lambda + \beta)y)^2 \; .$$

Thus

$$\langle F, \text{grad } \phi \rangle \geq \epsilon |F|^2$$

where $\epsilon = \min(1, 2\eta/c')$, so ϕ does indeed increase along the orbits of (7.4). For

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(7.3) we must compute $\langle \tau_x F, \mathrm{grad}\ \phi \rangle$. Let us write $\tau_x = \tau_0 + \tau_x'$, where τ_0 is the value of τ_x at the origin. Now τ_0 is a positive definite, diagonal matrix, and it is easily seen that

$$(7.7) \qquad\qquad \langle \tau_0 F, \mathrm{grad}\ \phi \rangle \geq \delta |\tau_x F|^2 ,$$

for some appropriately small positive δ. On the other hand $\langle \tau_x' F, \mathrm{grad}\ \phi \rangle$ vanishes to higher order at the origin and may be dominated by (7.7) in a sufficiently small neighborhood. This proves the above claim and thereby verifies the stability assignments made for the three cases I_0, III_0, III_1. (Incidentally since (7.4) admits a Lyapunov function, no Hopf bifurcation is possible for these cases. Cf. below.)

It remains to verify the stability assignments for the two cases I_1 and III_2, in which $c > 0$, $\eta < 0$. (The case $c < 0$, $\eta > 0$ does not occur for the problem at hand.) The bifurcation diagram

$$\{ (x, \lambda)\ :\ F(x, \lambda) = 0 \}$$

consists of two conic sections, one in the plane of symmetry $y = 0$ and one in the plane

$$(7.8) \qquad\qquad c'x + \lambda + \beta = 0 .$$

We refer to these as the symmetric and asymmetric solutions respectively. The stability properties of the symmetric solutions present no problem, because in the plane of symmetry τ_x and dF are diagonal matrices, the entries of τ_x being positive; thus the eigenvalues of dF and of $\tau_x \cdot dF$ are real and have the same signs. Our analysis of the asymmetric solutions is based on the following two facts, proved below. In these statements large only means close to the boundary of an appropriate neighborhood of zero.

(7.9) In case III_2, the asymmetric solutions are unstable for sufficiently large negative λ and stable for sufficiently large positive λ.

(7.10) At most one Hopf bifurcation is encountered along the asymmetric branches as λ is increased from large negative values to large positive values.

Assuming (7.9) and (7.10) the reader may verify our assignments of stability in the remaining diagrams of §2 by tracing the various solution branches in from large values of λ, using the principle of exchange of stability at bifurcation points. The essential idea here is that the stability assignment along a smooth branch of the bifurcation diagram can only change at a Hopf bifurcation point, and (7.10) provides the necessary control to show that there is a unique assignment possible. For example in Figure $2.4e_2$ no Hopf bifurcation is possible, while in Figure $2.4e_1$ a Hopf bifurcation is required. It should be mentioned that Figure $2.4b_1$ was drawn assuming $1 < c < 2$; a slightly different diagram results if $c > 2$, and we exclude the degenerate case $c = 2$ from consideration below.

Both (7.9) and (7.10) follow from the same estimates. On using (7.8) to eliminate x from the first equation in (3.6) we find that the asymmetric solutions lie on the conic section

$$(7.11) \qquad y^2 = \left(\frac{1}{c'^2} - \frac{1}{c'}\right)\lambda^2 + \frac{\beta}{c'}\lambda + \left(\alpha + \frac{\beta}{c'}\right) .$$

Now along the asymmetric solutions

$$dF = \begin{pmatrix} 2x + \lambda & -2y \\ c'y & 0 \end{pmatrix} .$$

Thus $\det dF = 2c'y^2 \geq 0$, so both eigenvalues have real parts of the same sign; the same statement holds for $\tau_x \cdot dF$, and we may determine the sign by examination of the trace. A trivial calculation yields

$$(7.12) \qquad \operatorname{tr} \tau_x \cdot dF = \tau_{11}(2x + \lambda) + \tau_{12}(cy) + \tau_{21}(-2y) .$$

We remind the reader that τ_{12} and τ_{21} are odd functions of y, so that the last two terms in (7.12) are $O(y^2)$. If we use (7.8) and (7.11) to eliminate x and y from (7.12) we find that

$$(7.13) \qquad \operatorname{tr} \tau_x dF = \tau_{11}\{(1 - \frac{2}{c'})\lambda + \text{hot}\}$$

where terms that are of order λ^2, α, or β are called higher order, as the first term in (7.13) will dominate the others if the parameters are appropriately restricted.

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In case III_2, we have $0 < c < 1$, so that the coefficient of λ in (7.13) is negative. Thus $\text{tr } \tau_x \cdot dF$ is positive for large negative λ, indicating eigenvalues with positive real part or instability as claimed in (7.9); and similarly for large positive λ. A Hopf bifurcation can occur only if (7.13) vanishes, which will happen for exactly one value of λ, say λ^*. If λ^* yields real solutions y in (7.11) the associated bifurcation diagram will possess a Hopf bifurcation point; otherwise not.

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In this paper we analyze the steady-state bifurcations from the trivial solution of the reaction-diffusion equations associated to a model chemical reaction, the so-called Brusselator. The present analysis concentrates on the case when the first bifurcation is from a double eigenvalue. The dependence of the bifurcation diagrams on various parameters and perturbations is analyzed. The results of Technical Summary Report #1844 are invoked to show that further complications in the model would not lead to new behavior.

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